Abstract Submitted
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Workflow Management Systems for Molecular Dynamics on Leadership Computers[1] JACK WELLS, Oak Ridge National Lab, SERGEY PANITKIN, Brookhaven National Lab, DANILA OLEYNIK, U. Texas-Arlington, SHANTENU JHA, Rutgers U. — Molecular Dynamics (MD) simulations play an important role in a range of disciplines from Material Science to Biophysical systems and account for a large fraction of cycles consumed on computing resources. Increasingly science problems require the successful execution of "many" MD simulations as opposed to a single MD simulation. There is a need to provide scalable and flexible approaches to the execution of the workload. We present preliminary results on the Titan computer at the Oak Ridge Leadership Computing Facility that demonstrate a general capability to manage workload execution agnostic of a specific MD simulation kernel or execution pattern, and in a manner that integrates disparate grid-based and supercomputing resources. Our results build upon our extensive experience of distributed workload management in the high-energy physics ATLAS project using PanDA (Production and Distributed Analysis System), coupled with recent conceptual advances in our understanding of workload management on heterogeneous resources. We will discuss how we will generalize these initial capabilities towards a more production level service on DOE leadership resources.

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